The Structure and Properties of Nanoporous Materials

The aim of the proposed research is to determine how the structure of highly porous metal and metal oxide foams changes with temperature, pressure, and surface environment. The research will also seek to understand how changes in the nanostructure of these foams alter their mechanical behavior. How these porous materials deform with thermal stresses and surface tension will be examined with a combination of Small Angle X-ray Scattering (SAXS) and high-resolution Synchrotron Radiation Computed Tomography (SRCT). Theoretical treatments of foam strength are based on the local stresses exceeding the yield strength in ductile metallic foams, or the flexural strength in brittle foams. However, these theories have never been tested at the densities and nanometer-length scales of the foams we propose to study.

Project Goals

Our goals are as follows:

1. High-spatial-resolution SAXS and SRCT measurements of the pore structure in metal oxide aerogels to determine the density, pore size, pore distribution, and aspect ratios of the cell backbone.
2. Extremely high-resolution diffraction imaging to determine the structure of the lattice of a select, low-density metal oxide foam and provide a basis for interpreting the SAXS data.
3. Finite-element modeling, using the structures determined in the first goal to study the effects of mechanical loading on the cell structures, and to map out relationships among processing, density, and strength. Thermal gradients, thermal stresses, and wetting will be explored.

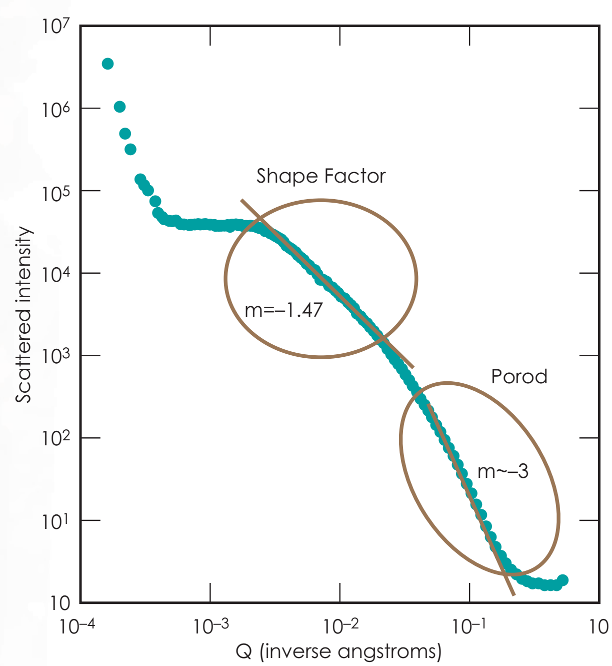

Figure 1. Image showing the scattering intensity as a function of the wave vector, Q. Shape factors and the slope of the Porod region are characteristic of a rod-like structure with rough surfaces.

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4. Determining the extent of any anisotropy in lattice architecture, and improving spatial resolution to characterize graded-density structures.

Relevance to LLNL Mission

This program develops critical experimental technologies for many LLNL applications. A key deliverable will be the ability to predict the mechanical properties of nanoporous materials and characterize gradient-density foam microstructures for future laser targets.

FY2005 Accomplishments and Results

Ultra-small-angle x-ray scattering (USAXS) was performed at the Advanced Photon Source on a 100-mg/cc tantalum oxide (Ta_2O_5) foam. The scattering as a function of wave vector, Q, is indicative of scattering from a collection of rod-like structures with a rough surface (Fig. 1). To get a complete understanding of the 3-D structure of the foam, a series of images were obtained using a lensless diffraction technique. The cell structure was determined from this image (Fig. 2).

The lensless images have enabled us to understand the meaning of the length scales determined from the USAXS experiments. We are confident that the USAXS data is providing us details about the cell size in these foams from 10 to 1000 nm.

We used a finite-element simulation to estimate the apparent elastic modulus of the foam structures using NIKE3D periodic boundary conditions. An apparent Young's modulus (E_s/E_b, where E_s is the modulus of the structure and E_b is the modulus of full-density Ta_2O_5) of 1.2×10^{-4} was determined. This is less than the value of 7.5×10^{-3} predicted from theory. However, theoretical models assume that all the mass is distributed within beams of uniform shape. An attempt was made to distinguish between mass associated with nodes and mass associated only with the beams. We established that, for the 100 mg/cc Ta_2O_5 foam, approximately 85% of the mass was confined to the nodes. Correcting the scaling laws for the reduced apparent mass lowered the theoretical estimate to 1.7×10^{-4}, in excellent agreement with the simulations.

FY2006 Proposed Work

We plan to continue the characterization of pore structure as a function of preparation condition for Ta_2O_5 and other metal oxide foams, and determine how the pore structure is affected by mechanical deformation. Also we will start the high-resolution density measurements on the graded-density materials.

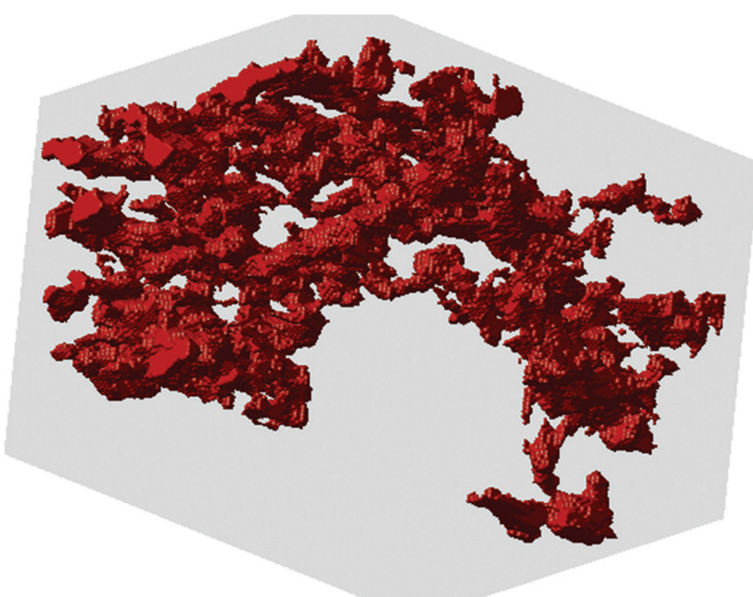

Figure 2. High-resolution reconstruction of a 500-nm cube from the interior of the foam (resolution 13 nm).